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Long-Range Order in a Quasi One-Dimensional Non-Equilibrium Three-State Lattice Gas

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Abstract. – Biased diffusion of two species with conserved dynamics on a $2 \times L$ periodic lattice is studied via Monte Carlo simulations. In contrast to its simple one-dimensional version on a ring, this *quasi* one-dimensional model surprisingly exhibits phase separation in its steady state, which is characterized by one *macroscopic* particle cluster. We study the order parameter and the cluster-size distributions as a function of the system size L , to support the above picture.

Driven diffusive lattice gases are among the simplest systems exhibiting generic non-equilibrium behavior in their steady states [1, 2]. Even the simplest group of these models with purely short-range interactions, produced by the excluded volume constraint, can display complex phase diagrams when driven away from equilibrium. The ones with non-trivial phase diagram typically involve a breaking of translational invariance (*e.g.*, open boundaries [3]), or more than one species of particles [4, 5]. The study of multi-species systems is also motivated by fast ionic conductors with several mobile species [6], water droplets in microemulsions with distinct charges [7], gel electrophoresis [8, 9], and traffic flow [10].

One striking feature of the non-equilibrium steady states of some of these models is that they exhibit spontaneous symmetry breaking or phase separation in *one dimension* (1D), in contrast to equilibrium systems with short-range interactions, where no long-range order (LRO) exists at finite temperature, *i.e.* with noise present. Indeed, a simple two species asymmetric exclusion model with *open boundaries* display the unusual phenomenon of spontaneous symmetry breaking in one dimension [11]. Also, phase separation, analogous to Bose condensation, triggered by defects has been observed in systems with *disorder*, related to simple traffic flow [12]. Recently, a quasi 1D model for the sedimentation of colloidal crystals [13], and a simple 1D “cyclic” three-state lattice gas [14], both homogeneous systems with no boundary effects (*i.e.*, with ring geometry), have been shown to undergo phase separation.

In this Letter we aim to illustrate that the role of dimensionality contributing to long-range order and the notion of “lower critical dimension” can be quite subtle in non-equilibrium systems. We focus on the difference between the 1D and the quasi 1D version of a driven three-state lattice gas, consisting of holes and two oppositely “charged” species of particles, subject to an “electric” field, E . *Particle-particle exchanges* (PPE) *are allowed* but occur on a much slower time scale than the dominant particle-hole exchanges. In two dimensions (2D), the system exhibits a transition from a disordered (homogeneous) to an ordered phase characterized by a compact strip of particles spanning the system transverse to the field [5]. Indeed, even in the *absence* of PPE, a phase transition exists [4]. In one dimension, the behavior of a system without PPE is clearly trivial. With PPE, it was first believed that the 1D system would mimic those in higher dimensions and display a transition to an ordered state. However, an exact solution (with $E = \infty$) was subsequently found [15], showing that this system *never* orders (though it exhibits non-trivial cluster size distributions [15] and microscopic shocks [16]). This behavior seems counter-intuitive, since blockages, which cause the transition to an ordered state, should be enhanced in a 1D system. On closer examination, blockages are found to be “over-enhanced”, in the sense that they occur on microscopic length-scales and prevent the macroscopic cluster from growing. As a result, the steady state of the 1D system is characterized by a typical particle cluster size, which depends only on the microscopics [15] and does not scale with the system size.

For *equilibrium* systems with short-range interactions, LRO cannot exist in a 1D chain or in a (quasi 1D) pair of chains. In contrast, the behavior of our model is much more intriguing. Using Monte Carlo simulations and simple theoretical methods [5], we investigate the steady states of a 1D system of L sites and the quasi 1D case of $2 \times L$. Confirming that there is no LRO in the 1D case, we find that the $2 \times L$ system behaves as an $L \times L$ one! In other words, a macroscopic cluster forms for sufficiently large E and particle density, with density profiles resembling the mean-field ones closely. For maximal effects, we choose $E = \infty$, so that we can compare directly with the exactly solvable model in 1D [15]. We have also considered a range of transverse diffusion rates, as a further attempt to interpolate between the ordering, $2 \times L$ system and the non-ordering 1D case.

A concise specification of our model consists of a (quasi 1D) periodic lattice of $2 \times L$ sites. A site $\mathbf{x} = (x, y)$ can be empty or occupied by either a positive or a negative particle. Associated with these occupancies are the standard variables $n_{\mathbf{x}}^+$, $n_{\mathbf{x}}^-$, which assume the value 0 or 1. The excluded volume constraint also implies $n_{\mathbf{x}}^+ n_{\mathbf{x}}^- = 0$, for any \mathbf{x} . The external field is chosen so that a positive (negative) particle *never* moves in the $-y$ ($+y$) direction. At each elementary time step, a pair of neighboring sites (“bond”) is chosen randomly. For an “ x -bond”, particle-hole pairs are exchanged with rate Γ_{\perp} , while PPE occurs with rate $\gamma \Gamma_{\perp}$. Similarly, for “ y -bonds”, the rates of the *allowed* exchanges are Γ_{\parallel} and $\gamma \Gamma_{\parallel}$, respectively. Note that γ sets the time scale for PPE processes. In the simulations presented here, $\Gamma_{\perp} = \Gamma_{\parallel} = 1$, $\gamma = 0.10$. As indicated, we also studied cases with $\Gamma_{\perp}/\Gamma_{\parallel} < 1$, since the $\Gamma_{\perp} = 0$ limit corresponds to two uncoupled 1D systems. Our time unit is one Monte Carlo step (MCS), during which $4L$ bonds are chosen. We also restrict ourselves to “neutral” systems ($\sum_{\mathbf{x}} n_{\mathbf{x}}^+ = \sum_{\mathbf{x}} n_{\mathbf{x}}^-$) at half filling, *i.e.*, $\overline{m} \equiv \frac{1}{2L} \sum_{\mathbf{x}} (n_{\mathbf{x}}^+ + n_{\mathbf{x}}^-) = 0.5$. On lattices with L ranging from 10^2 to 10^4 , our runs last from 5×10^5 to 2×10^6 MCS. Averages, denoted by $\langle \dots \rangle$, are performed over the time series, once the system has settled in a steady state. To ensure that the final state is independent of the initial configuration, we started the simulations with both disordered (random) and fully ordered configurations.

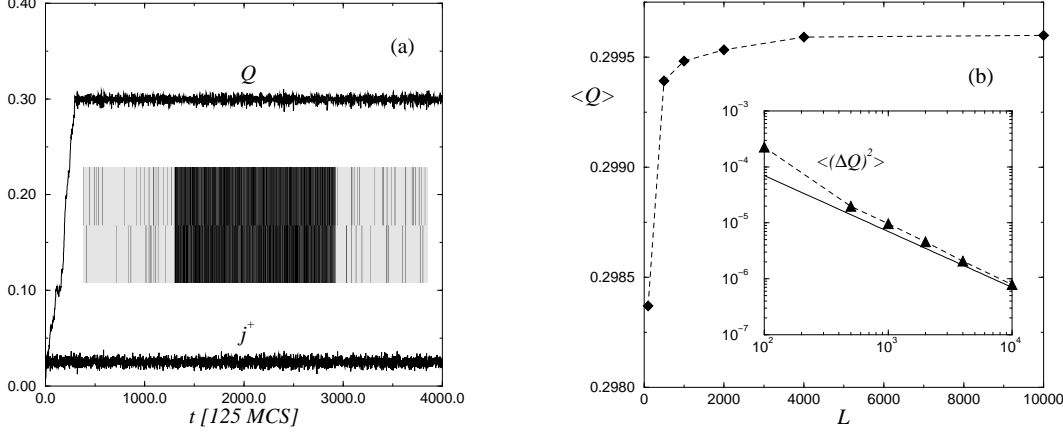


Fig. 1. – (a) Time-series of Q and j^+ for $L = 1000$, starting from random initial configuration. The inset shows a typical ordered configuration for the same L (bias points to the right); black, dark gray, light gray corresponds to +’s, –’s, and holes respectively. (b) Finite-size effect for $\langle Q \rangle$ and $\langle (\Delta Q)^2 \rangle$ (inset) in the ordered phase. The solid line in the inset represents a $1/L$ power law. Note the extremely small change in $\langle Q \rangle$ (less than 0.5% of its saturation value).

To characterize the steady state, we define the particle density profile (in y):

$$\rho(y) = \frac{1}{2} \sum_{x=1}^2 (n_{xy}^+ + n_{xy}^-) \quad (1)$$

and an (unnormalized) order parameter,

$$Q = \left| \frac{1}{L} \sum_{y=1}^L e^{i2\pi y/L} \rho(y) \right|, \quad (2)$$

Being the magnitude of the lowest Fourier component of ρ , Q provides a sensitive measure of the density inhomogeneities. For the completely ordered configuration (*i.e.*, $\rho = \Theta(\overline{m}L - y)$; Θ being the Heaviside step-function), $Q = \sin(\overline{m}\pi)/(L \sin(\pi/L)) \approx 0.318$ for an infinite system with $\overline{m} = 0.5$. On the other hand, $\langle Q \rangle$ vanishes in the disordered phase, up to finite size effects of $\mathcal{O}(1/\sqrt{L})$. We measured j^+ , the current of positive particles. By symmetry, the average negative particle current should be just $-\langle j^+ \rangle$. Finally, we also constructed size distributions for both particle and hole clusters by building histograms with respect to their length along the field in one fixed “column”, say for $x = 1$.

For all of our system sizes, we observed that the steady-state configuration is ordered (inset of fig. 1a). Most of the particles “condense” into one *macroscopic* cluster, while the remainder scatters as a small but finite density of “travellers” through the empty region. Due to the infinite field, holes cannot enter the macroscopic particle cluster. Note that there will always be a *finite* current of either species (proportional to γ) in the system, so that coarsening does take place. The growth of this cluster, when the initial configuration is random, is quite interesting. After the first 10-20 MCS, small blockages (particle clusters) form everywhere. After this initial phase, a somewhat slower process takes over: particle clusters coarsen in time until a single, macroscopic cluster remains in the system. The evolution of Q (fig. 1a)

provides a good picture of this growth process. One important observation is that the value of the current is basically unaffected after the initial appearance of small clusters throughout the coarsening process (fig. 1a). This can be understood: the current is mainly controlled by PPE within the bulk of the particle clusters.

Taken alone, the appearance of a single large cluster is not sufficient for us to conclude the presence of an ordered state. Indeed, even for the 1D case, in which there is a finite typical particle cluster size ($l_p^* \sim 4\gamma^{-2}$ for $\bar{m} = 0.5$) [15], we would generally observe a single cluster if $L \ll l_p^*$. Although the range of our L 's does exceed $4\gamma^{-2} = 400$, we probe more deeply by analyzing the L dependence of various quantities. The conclusion is that, if $\gamma L^\omega \gtrsim 1$ were the criterion for the $2 \times L$ system to display 1D behavior, then $\omega \simeq 0$. In other words, we believe that the collective properties of the quasi 1D system are distinct from the non-ordering 1D chain, but fall within the class of the higher dimensional systems. In the remainder of this letter, some details of our analyses are provided.

In fig. 1b, we show the average order parameter, $\langle Q \rangle$, as a function of L . It saturates rapidly; even with $L = 100$, it is within 0.5% of the apparent $L = \infty$ limit. Meanwhile, its fluctuations, $\langle (\Delta Q)^2 \rangle = \langle Q^2 \rangle - \langle Q \rangle^2$, decay like $1/L$ (inset fig. 1b). The distribution of the sizes of *particle* clusters reveals more of the nature of the steady state. Denoting by $P(l, L)$ the probability of finding a cluster of length l in a system of size L , we are not surprised that there are two well-separated components, one corresponding to the single macroscopic cluster and the other to the small clusters of “travellers”. The macroscopic component appears as a peak at l_0 . We found that $l_0 \approx 0.471L$, which is a result of $\bar{m} = 0.5$ and a clear signal of the large cluster scaling linearly with the system size. Meanwhile, δl_0 , the standard deviation, grows as \sqrt{L} . Focusing on this component alone, we renormalize its integral to unity and rewrite it in terms of $u \equiv (l - l_0)/\delta l_0$. The result, $p(u, L)$, is well fitted by a Gaussian (fig. 2a). Deviations from the Gaussian, seen especially for small L , carry non-trivial information on finite size effects which should be investigated further. In the “travellers” component, the distribution decays exponentially ($\propto e^{-l/\lambda}$), with $\lambda < 1$ and *independent* of L . Similarly, the size distribution of the *hole* clusters is also a simple exponential, independent of L apart from finite size effects. Both of these exponentials can be understood [17] from the observation that the small density of “travellers” is roughly homogeneous. Following approaches to the percolation problem [18], we consider another interesting distribution, namely, the probability that a randomly selected particle belongs to a cluster of length l (at a given time). Clearly proportional to $lP(l, L)$, it will be referred to as the “residence” distribution. To compare distributions from different L 's, we define $w \equiv l/(\bar{m}L) \in (0, 1]$. Thus, $\tilde{P}(w, L)$ is the probability (density) that a particle “resides” in a cluster of length $w\bar{m}L$. Since there are essentially no holes in the particle clusters, w is just the fraction of all the particles in such a cluster. In fig. 2b, we see that $\tilde{P}(w, L)$ peaks at approximately 0 and at $w_0 \approx 0.942$. The areas under each component are essentially independent of system size, while both sharpen with increasing L . With finite L , the former peaks at $1/(\bar{m}L)$, with area 0.058. Of course, the complement area is under the other component. It is not a coincidence that this area (0.942) is identical to the peak position, w_0 , since both are simply related to the fraction of particles in the macroscopic cluster. Finally, note that this quantity is also $l_0/(\bar{m}L)$.

We also studied the system with varying transverse hopping rates: $0 \leq \Gamma_\perp/\Gamma_\parallel \leq 1$. Our results indicate that a crossover to the 1D behavior occurs at a very small but *finite* value of this ratio (of the order of 10^{-3}); only a very careful finite-size analysis could reveal whether this occurs when the transverse hopping rate becomes comparable to the inverse relaxation time of the 1D system.

Most of our data can be understood by simple mean-field considerations [5]. As we already pointed out, the current of one species (*e.g.*, that of the +’s) is controlled by the bulk of

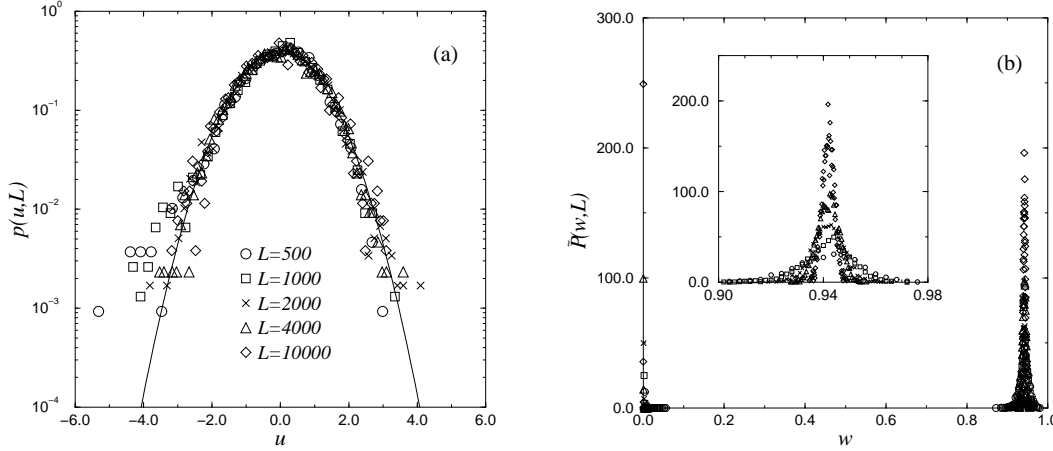


Fig. 2. – (a) The distribution of the relative size-fluctuations of the macroscopic particle clusters for different system sizes. The solid line is a Gaussian with zero mean and unit standard deviation. (b) The scaled residence distributions. System sizes and symbols are the same as in (a). The inset gives a closer view of the distribution around $w_0 = 0.942$.

the particle cluster. Although there is a non-trivial charge distribution within the particle cluster [17], it is fairly flat (up to finite size effects) around the *center* of the cluster: thus at the simplest level we can approximate the density of both species there to be equal to $1/2$, and $\langle j^+ \rangle \approx \gamma/4$. Since the steady state is stationary, the current must be constant and homogeneous through the system, so that $\langle j^+ \rangle \approx \gamma/4$ outside the particle cluster as well. Assuming a homogeneous density of “travellers”, m^* , outside the macroscopic particle cluster, we have [5] $\gamma/4 = (m^*/2)[(1 - m^*) + \gamma(m^*/2)]$, yielding $m^* = \gamma/(2 - \gamma)$. For $\gamma = 0.1$, $m^* = 0.0526$, which is within 5% of the Monte Carlo value. The mean macroscopic cluster size l_0 can also be deduced, since $l_0 + m^*(L - l_0) = \overline{m}L$. The result, $0.472L$, is very close to the one obtained from the measured particle cluster size distributions. Also, the order parameter for such an ordered configuration is just $Q = 0.30$, which compares well with the data (fig. 1a). Since the velocity of a tagged particle is approximately $\gamma/2$ in the particle cluster and $(1 - m^*) + \gamma(m^*/2)$ outside the cluster, it is easy to show that the typical time it spends diffusing through the macroscopic cluster is a fraction $l_0/(\overline{m}L)$ of the total time needed to travel through the system once. Thus, for our parameters, a randomly selected particle is found with probability 0.944 in the large particle cluster, which reproduces the location of the second peak of the distribution $\tilde{P}(w, L)$ quite well.

In summary, we have studied the non-equilibrium steady state of a driven, quasi one-dimensional, three-state stochastic lattice gas, using simulations and simple mean-field arguments. We found that, for the parameter regime studied, the properties of a *coupled pair* of chains of length L are drastically different from those of the strictly 1D system, *i.e.*, the single chain. With as little as 1% of cross-chain (transverse) moves, the $2 \times L$ model already develops a single macroscopic blockage, similar to the 2D ($L \times L$) system. Moreover, the finite-size analysis of the ordered phase, up to $L = 10^4$, shows no indication of a crossover to 1D behavior. Thus, we conjecture that LRO survives the $L \rightarrow \infty$ limit in our simple model (fixed γ and $\Gamma_\perp = \Gamma_\parallel$). If this conjecture proves to be true, our model would pose a stark contrast to, *e.g.*, the $M \times L$ equilibrium Ising model where LRO does not exist in the fixed

$M, L \rightarrow \infty$ limit. Instead, the strictly one-dimensional system is a “singular limit”, in much the same way that entirely different behaviors are found, obviously, in $1 \times L$ vs. $2 \times L$ systems of biased diffusion of two species *without* particle-particle exchange in finite field. The key difference between the strictly and the quasi 1D systems appears to be the ease with which particles can pass one another, leading to the formation of a macroscopic cluster. Work is in progress to reveal further differences between the 1D and the quasi 1D systems, *e.g.*, details of the coarsening process leading to LRO [17].

Note Added. – After submitting our manuscript we became aware of the work by Arndt *et al.* [19]. They studied a 1D model on a ring, similar to ours, but with different exchange rates.

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